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Towards mechanism-based simulation of impact damage using exascale computing

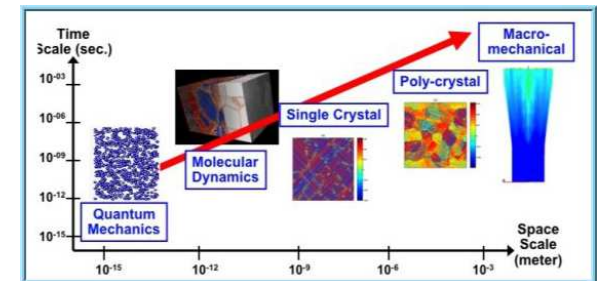
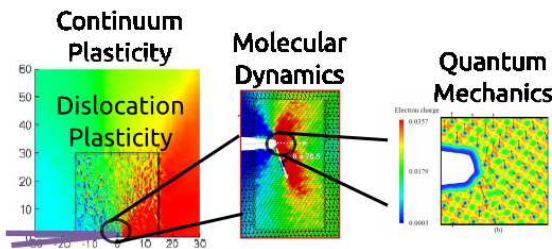
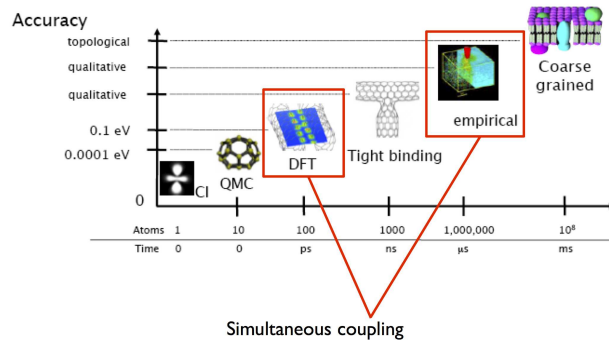
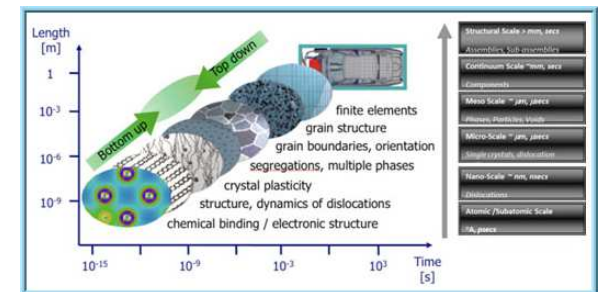
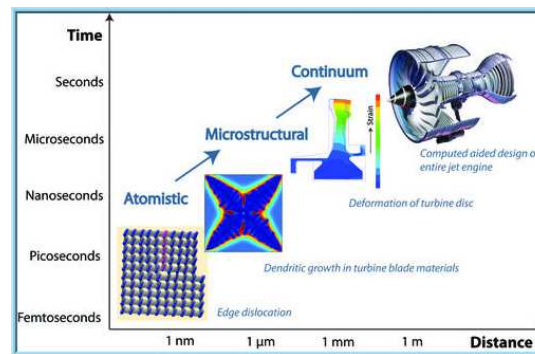
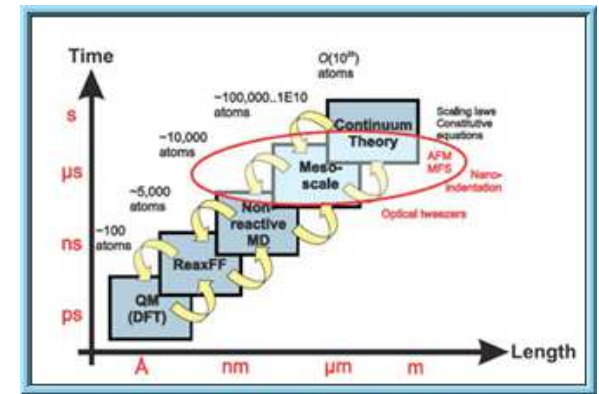
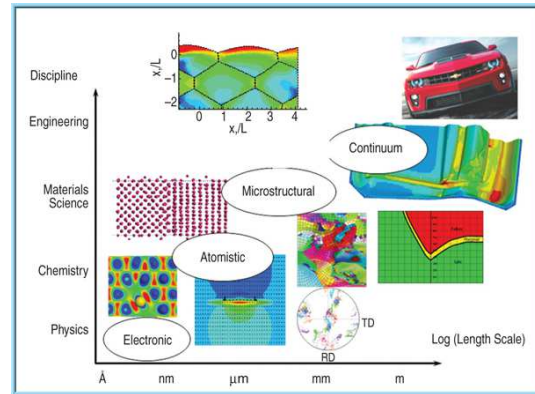
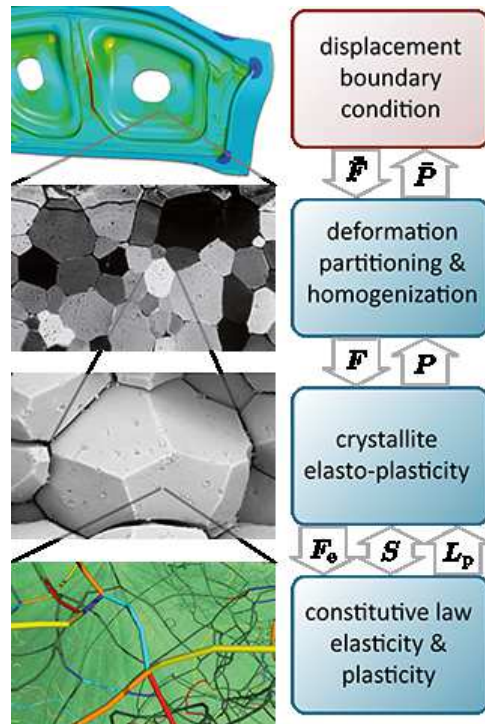
Anton Shterenlikht¹, Lee Margetts², Samuel McDonald², Neil Bourne²

¹The University of Bristol, UK

²The University of Manchester, UK



1. Multi-scale framework



2. Trans-granular cleavage

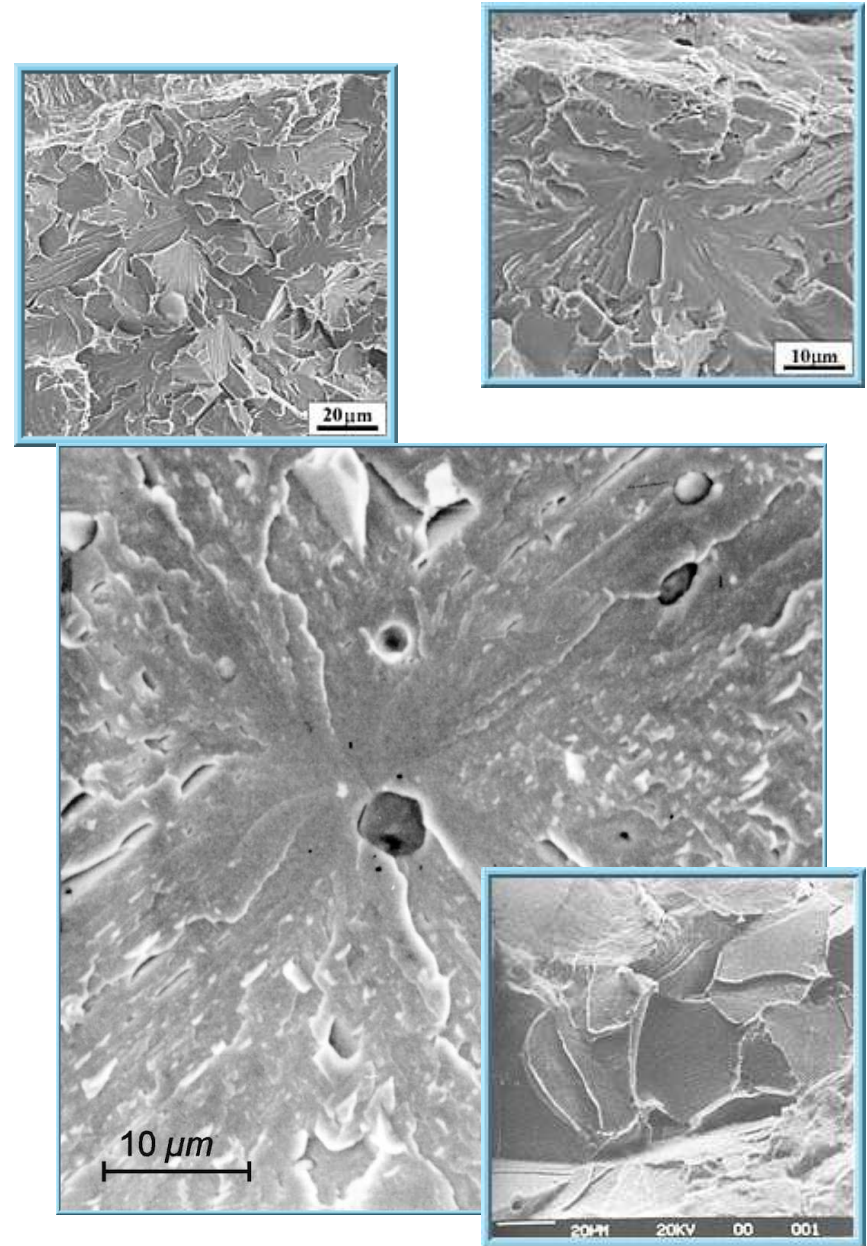
- \mathbf{t} - Macro stress tensor
- t - Resolved normal stress on crystal planes
- bcc crystals: $\{100\}$, $\{110\}$ planes cleave, normals \mathbf{n}_{100} , \mathbf{n}_{110}
- 24 planes of each family
- $t_{100}^{\max} = \max_{i=1 \dots 24} (\mathbf{n}_{100}^i \cdot \mathbf{t} \cdot \mathbf{n}_{100}^i)$
 $t_{110}^{\max} = \max_{i=1 \dots 24} (\mathbf{n}_{110}^i \cdot \mathbf{t} \cdot \mathbf{n}_{110}^i)$

Two parameters

- σ_F - critical stress, linked to γ , surface energy
- L - characteristic length, linked to wave speed, c .

Cleavage criterion

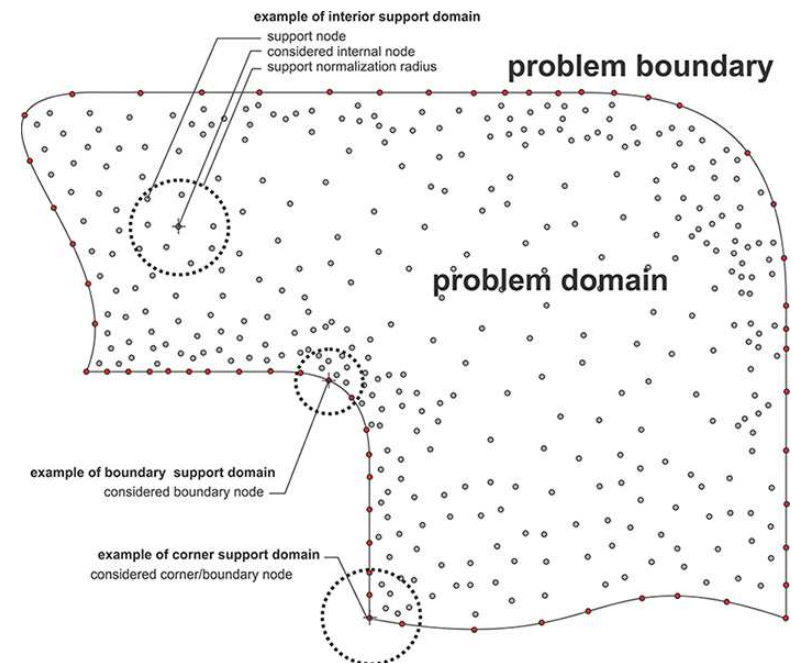
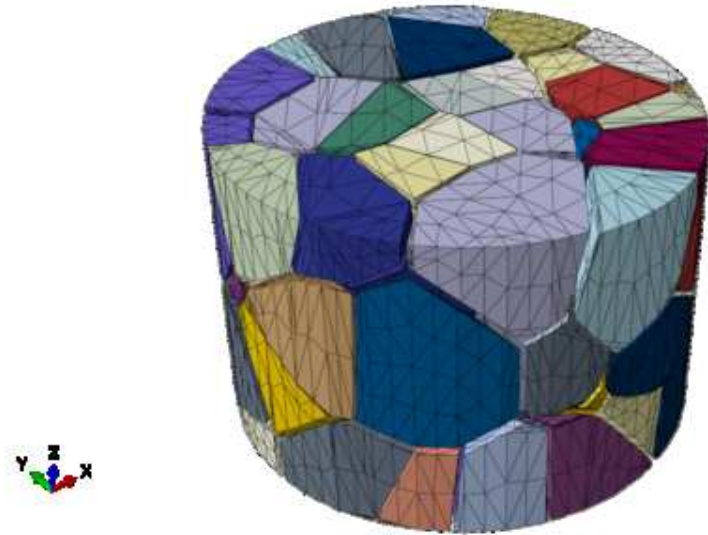
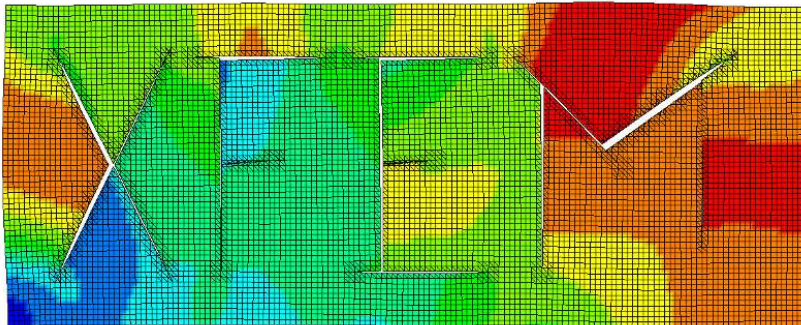
If $t_{100}^{\max} \geq \sigma_F$ or $t_{110}^{\max} \geq \sigma_F \rightarrow$ cleavage propagation over L per unit of time.



(Source: Internet)

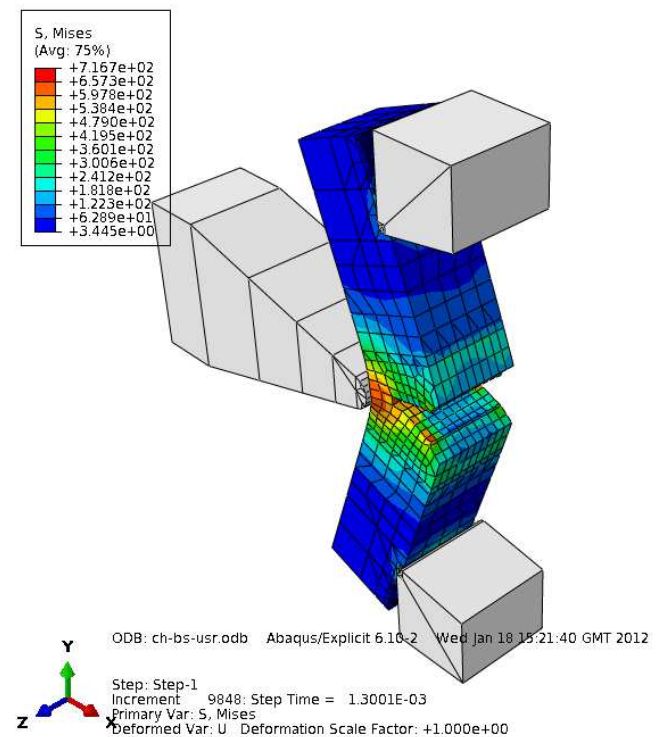
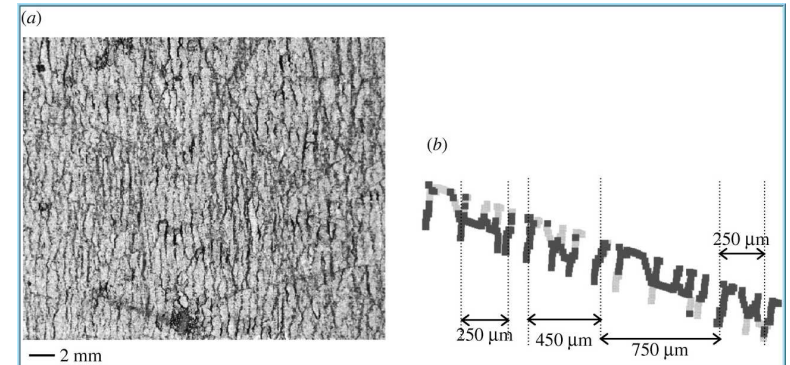
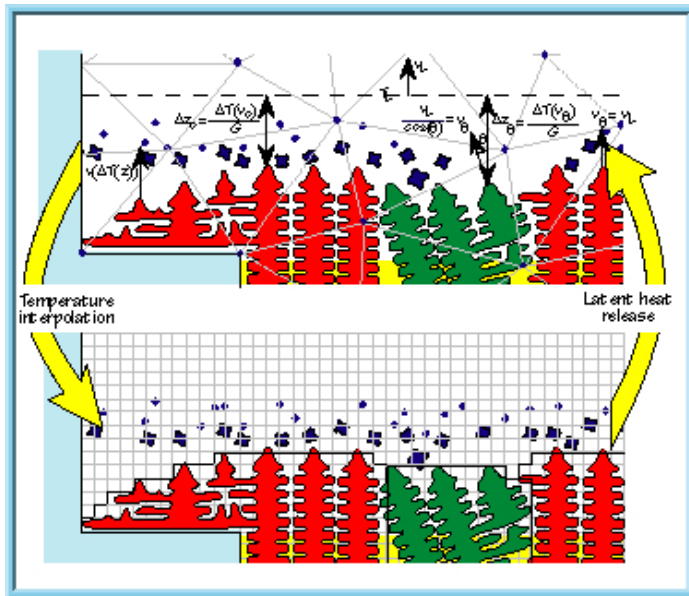
3. Multi-scale methods

- Coupled discrete dislocation and continuum plasticity¹
- Voronoi polyhedra FE²
- X-FEM³
- Element-free Galerkin (reproducing kernel particle)⁴
- Finite point⁵
- Free mesh⁶
- Meshless FE⁷
- Atomistic/continuum mech.⁸
- MD/continuum mechanics⁹



4. Cellular Automata Finite Element (CAFE)

- Used for solidification,¹⁰ recrystallisation¹¹ and fracture^{12, 13}
- FE - continuum mechanics - stress, strain, etc.
- CA - crystals, crystal boundaries, cleavage, grain boundary fracture
- FE \rightarrow CA - stress, strain
- CA \rightarrow FE - damage variables



5. Open source FE

ADVENTURE

Aladdin

ALBERTA

CalculiX

CMISS

Code_Aster

deal.II

DOUG

DUNE

Elmer

FEA(S)T

FENICS

FELIB

FElt

FELYX

FEMLISP

FEM_Object

FEMOCTAVE

FEMSET

FFEP

freeFEM

Getfem++ HMD

Impact

IMS

kaskade

KFEM

LUGR

MiniFEM

MODFE

MODULEF

NASTRAN

NLFET

OLEFI

OOFEM

Open FEM

Open FEM
(INRIA)

OpenSees

Padfem2

ParaFEM

Rheolef

SLFFEA

Sundance

TOCHNOG

VAPAS

VECFEM3

WARP3D

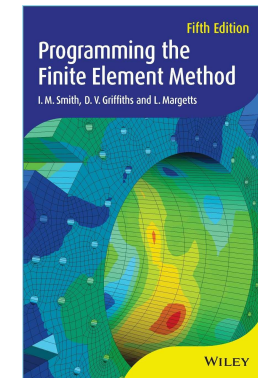
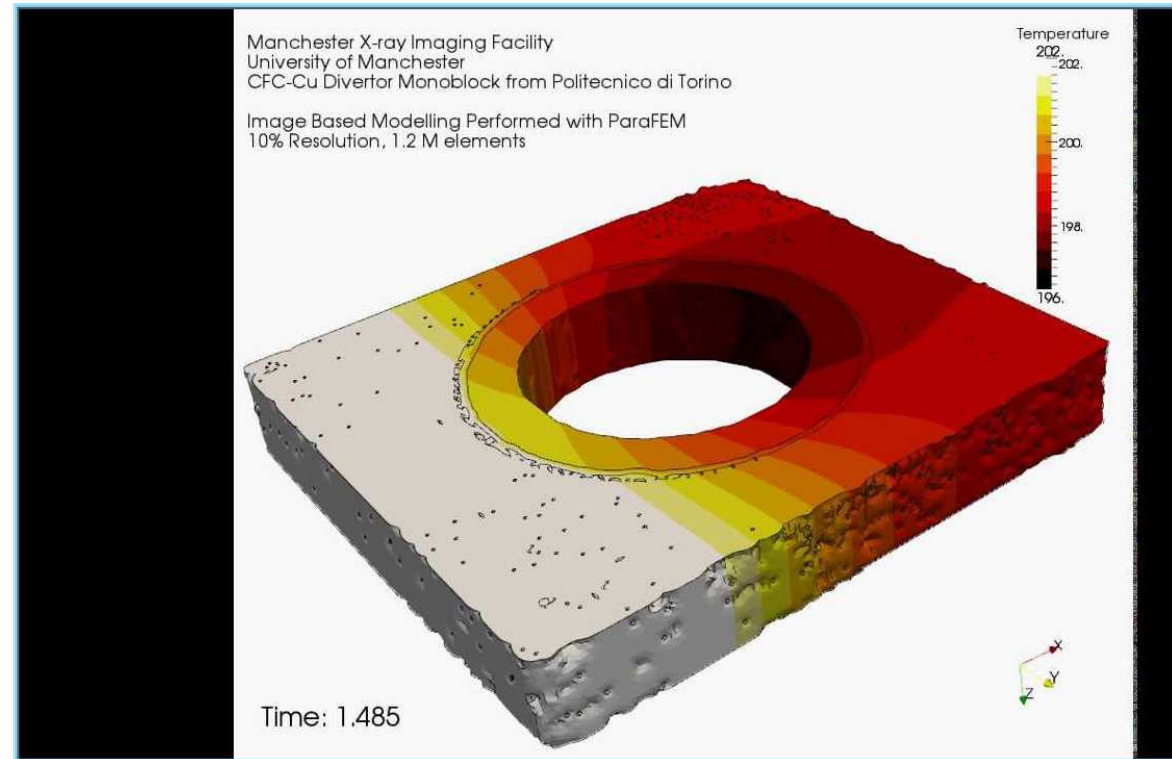
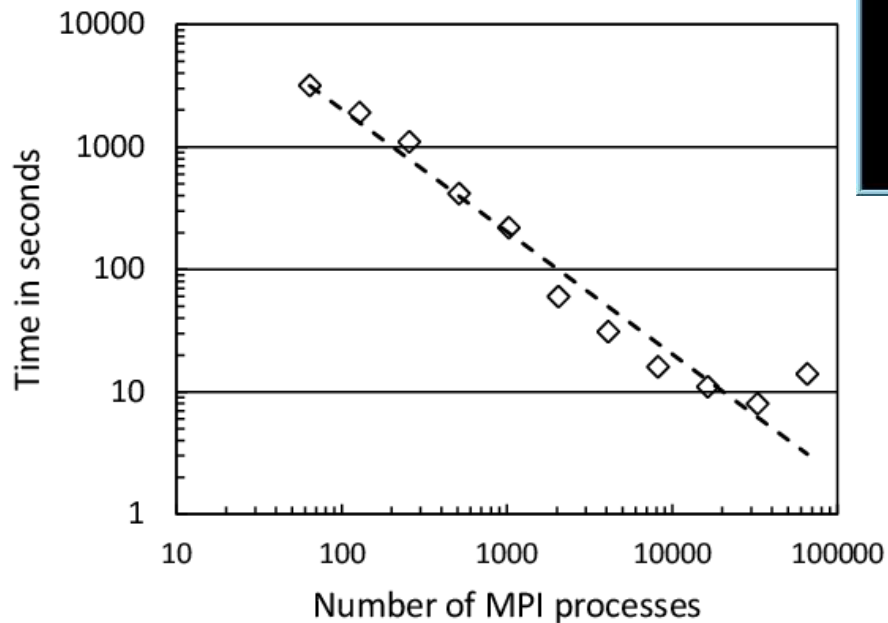
Z88

Problems

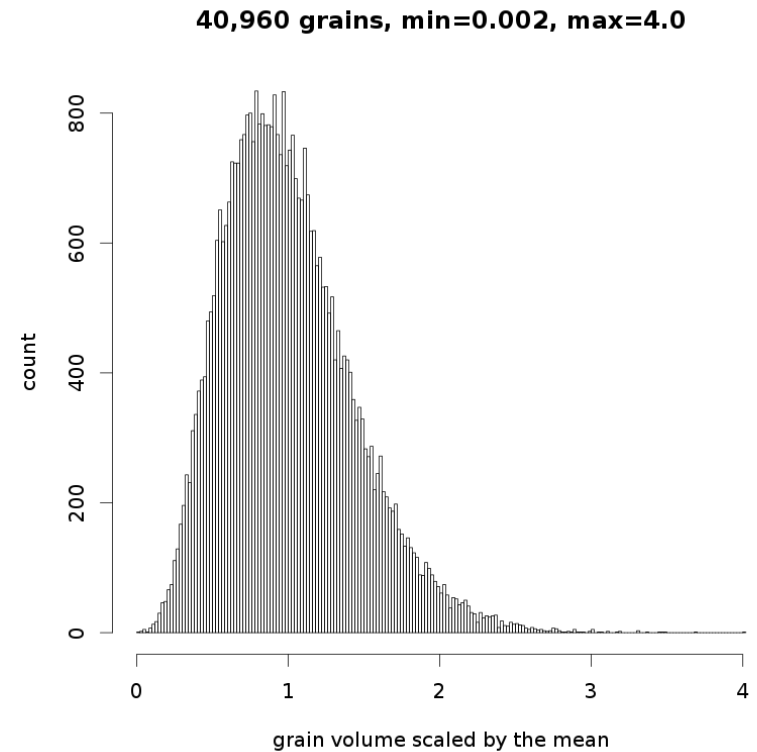
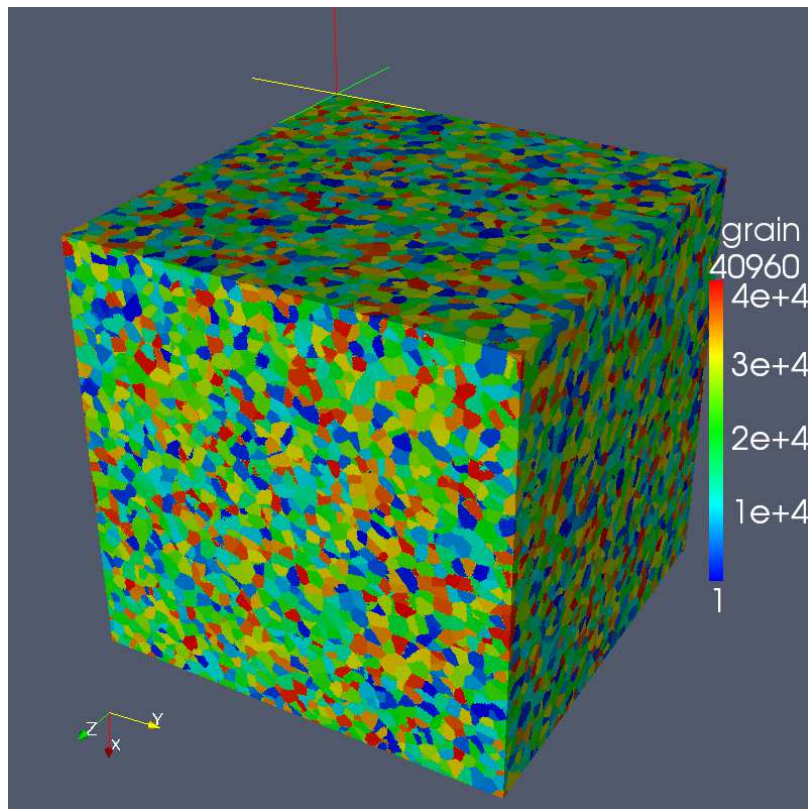
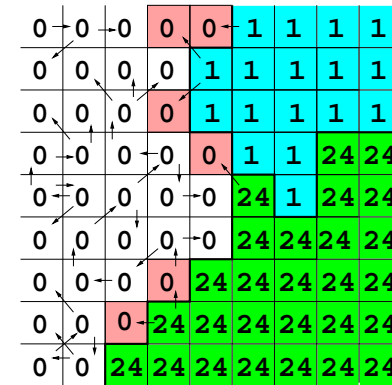
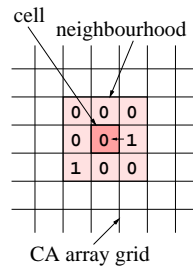
- Scaling
- Portability
- Documenta-
tion
- Flexibility
- Continuing
development
and future
proofing
- Standard
libraries
- Algorithms

6. ParaFEM¹⁴

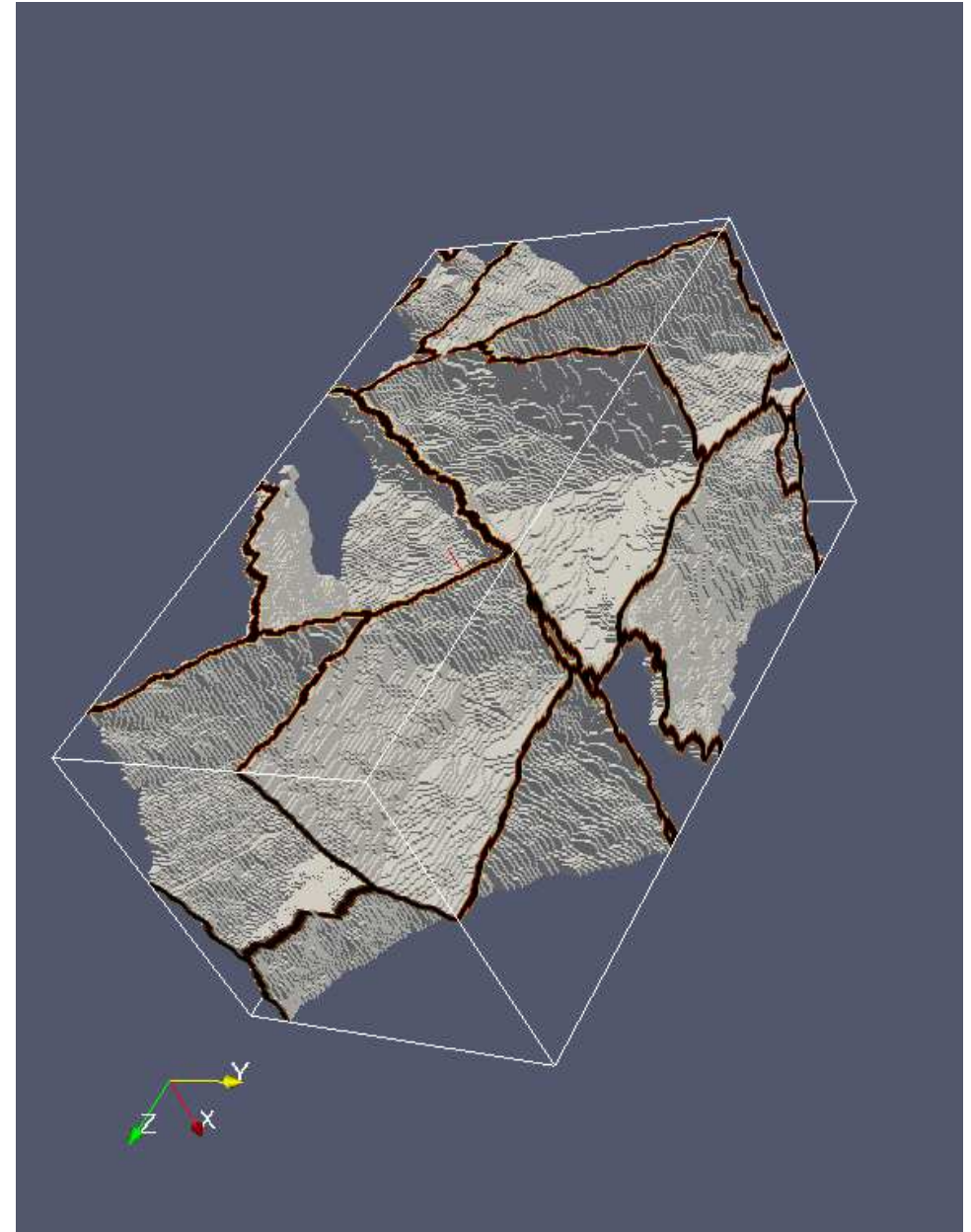
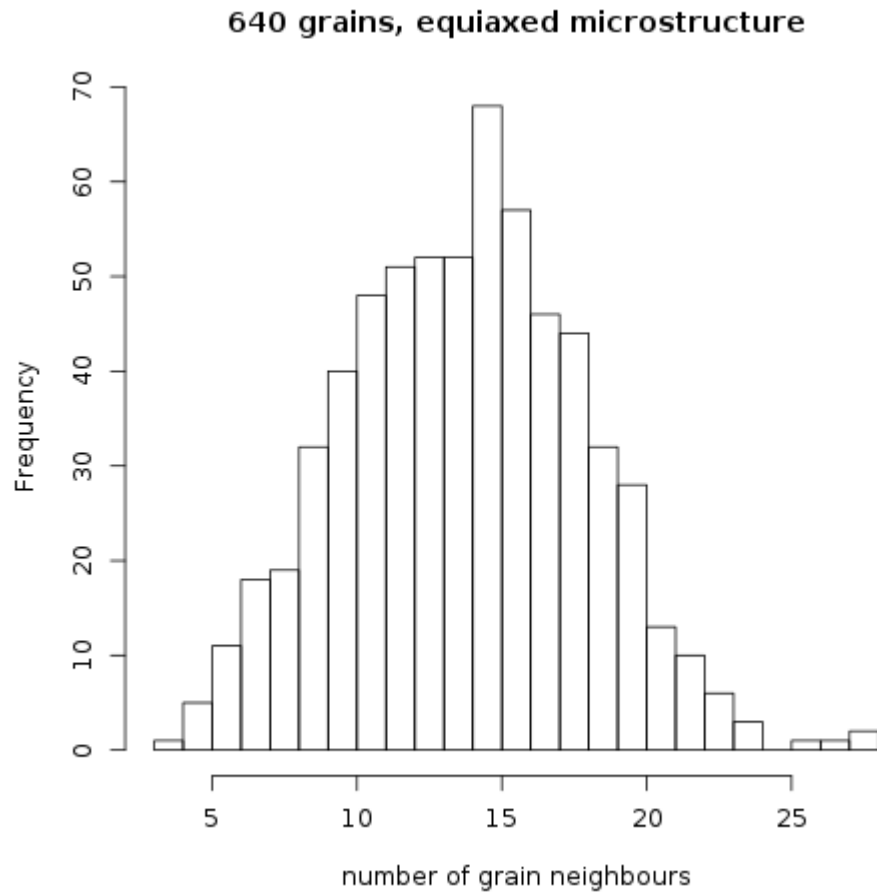
- MPI FE library
- Solids, fluids, heat transfer, dynamics, modal
- Highly scalable, >50k cores
- >125M elements
- parafem.org.uk



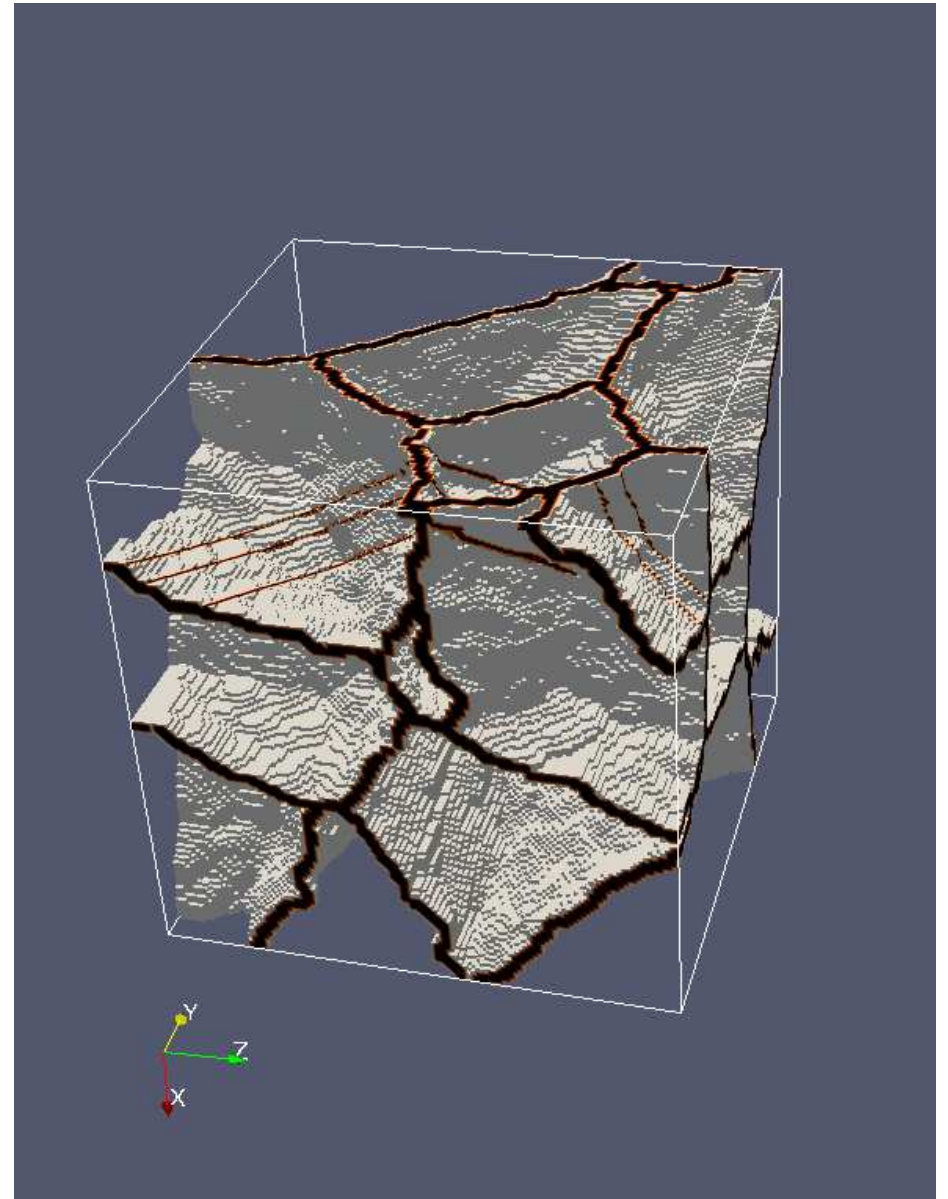
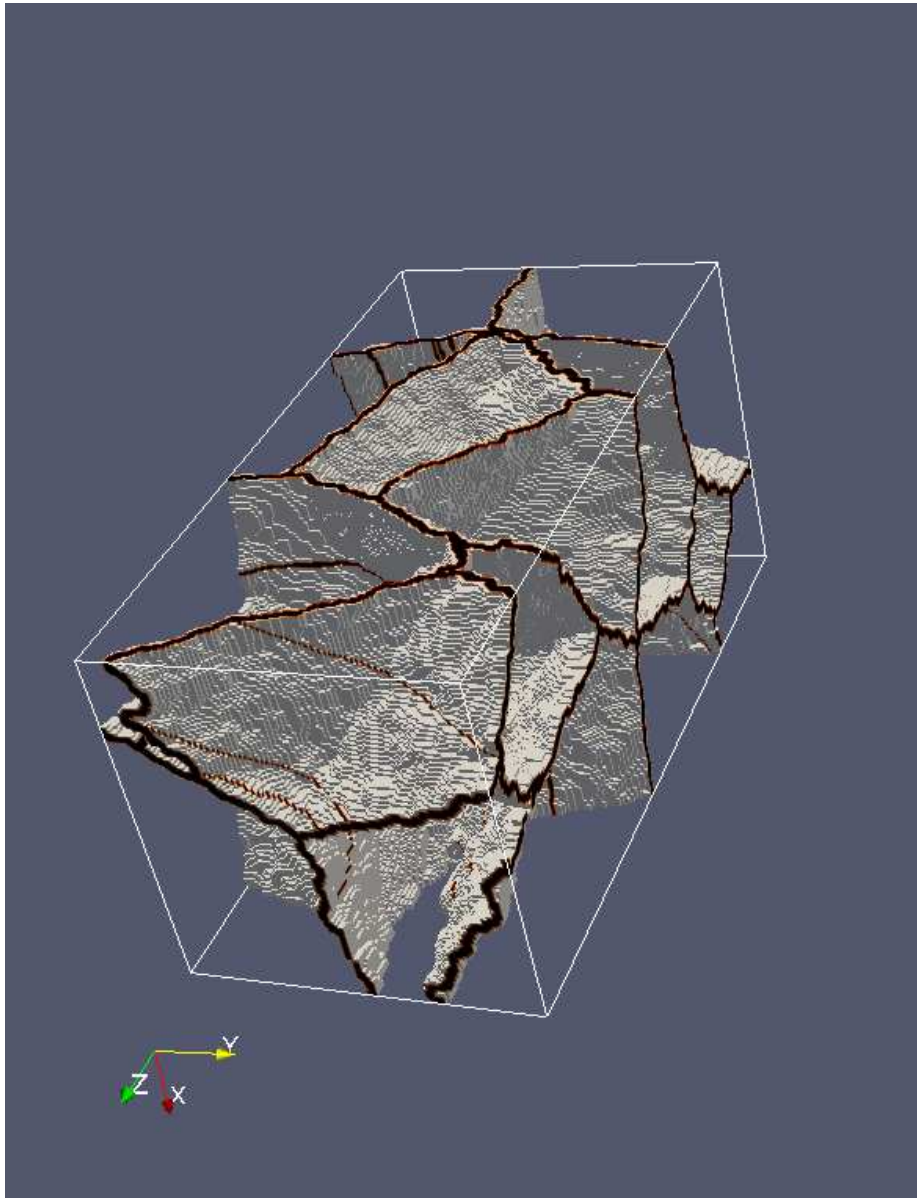
7. CGPACK^{15, 16, 17} - Cellular automata for polycrystals



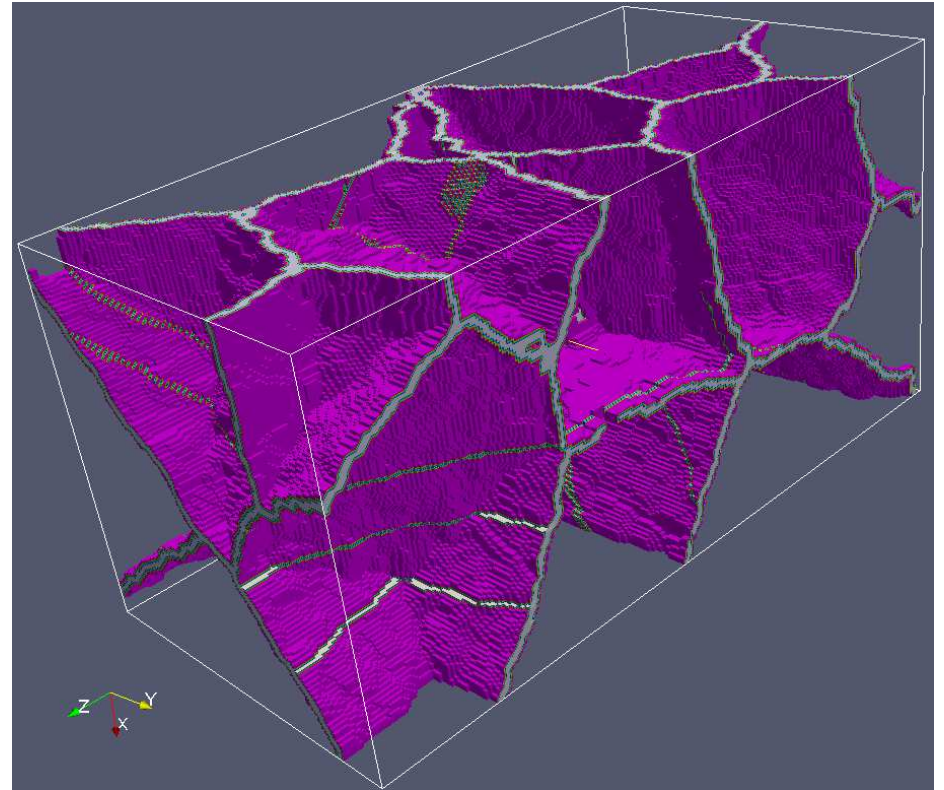
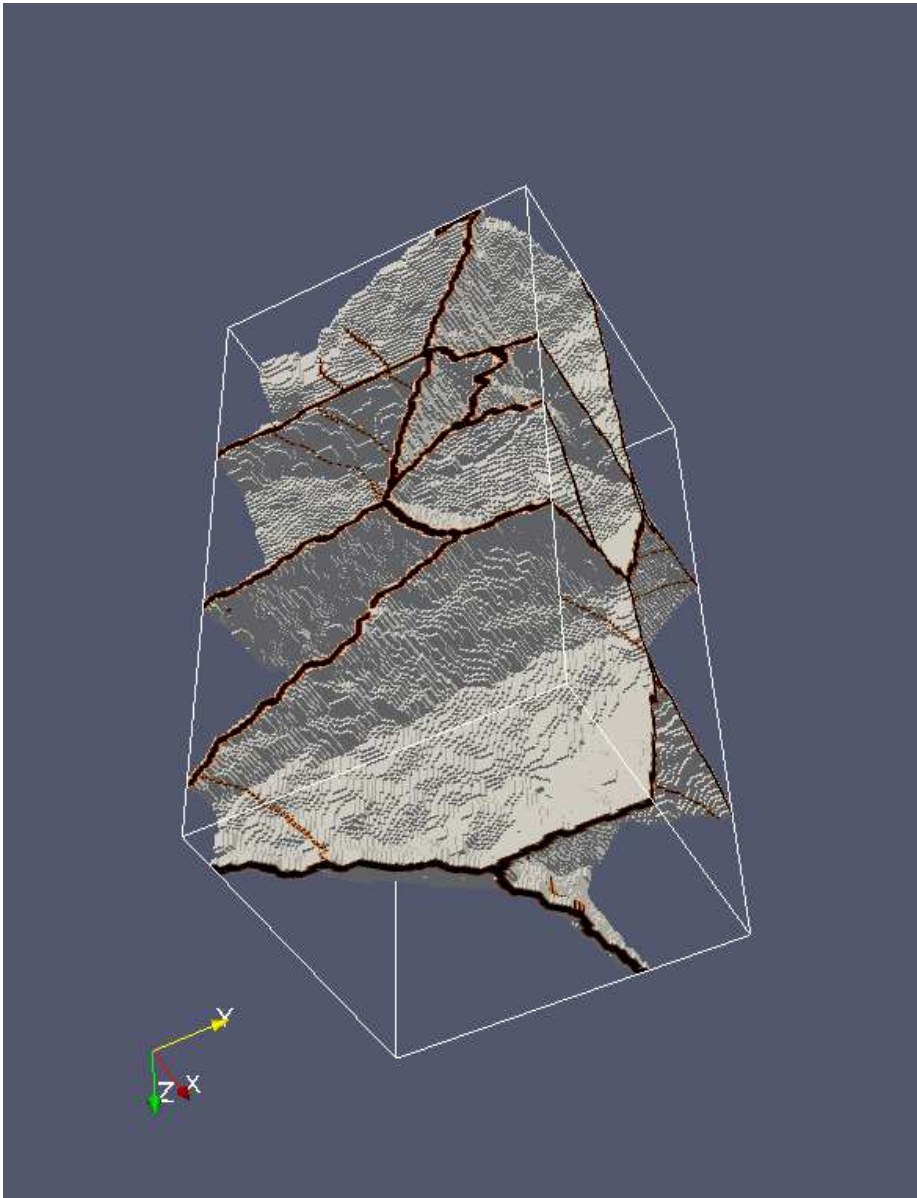
8. Grain boundaries



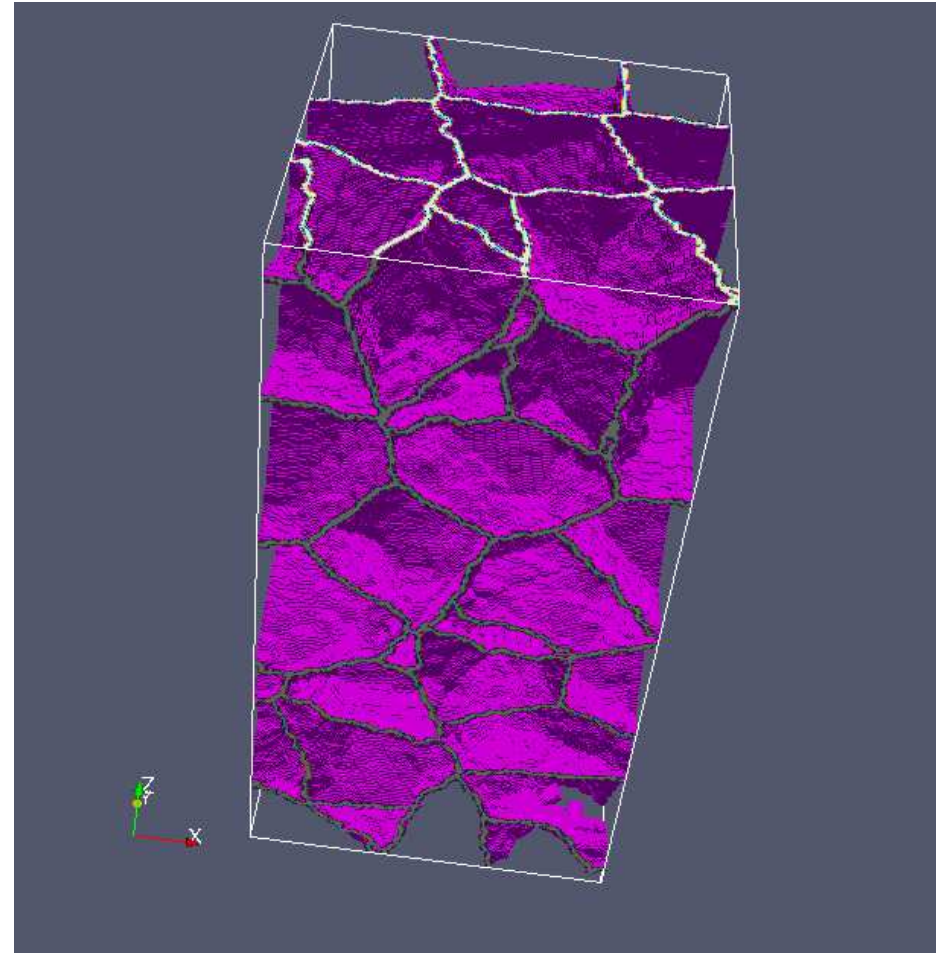
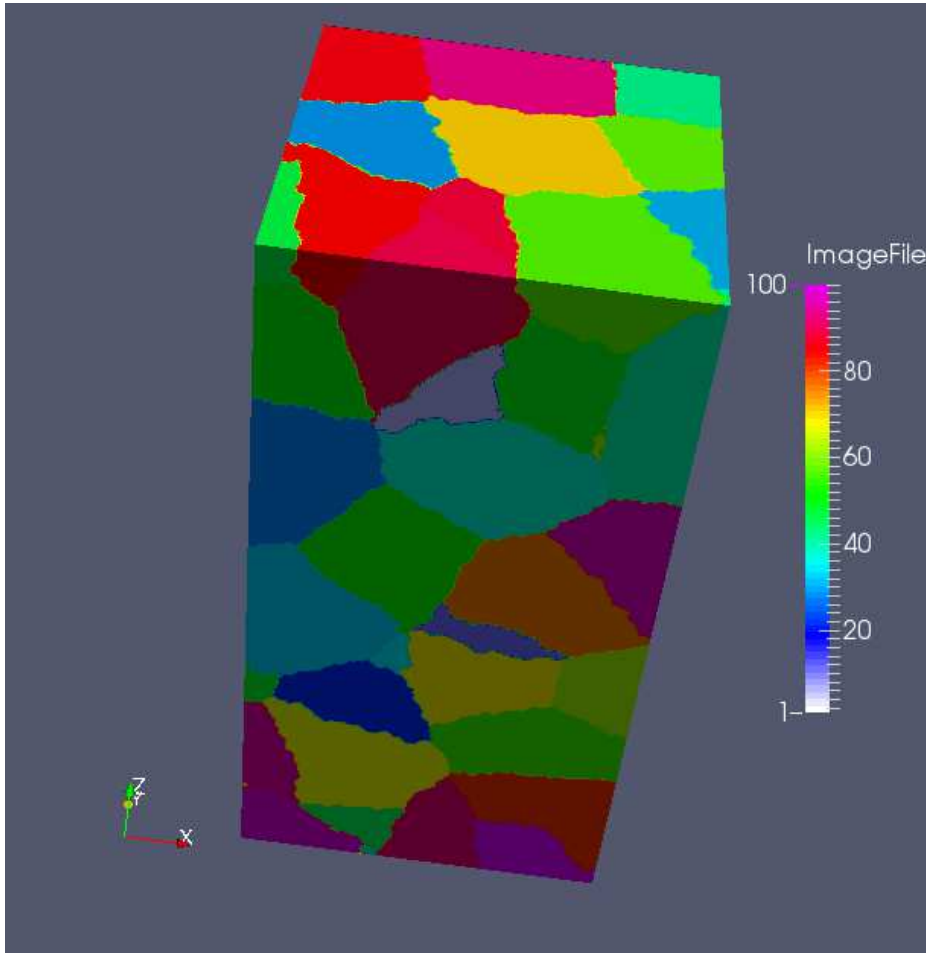
Grain boundaries



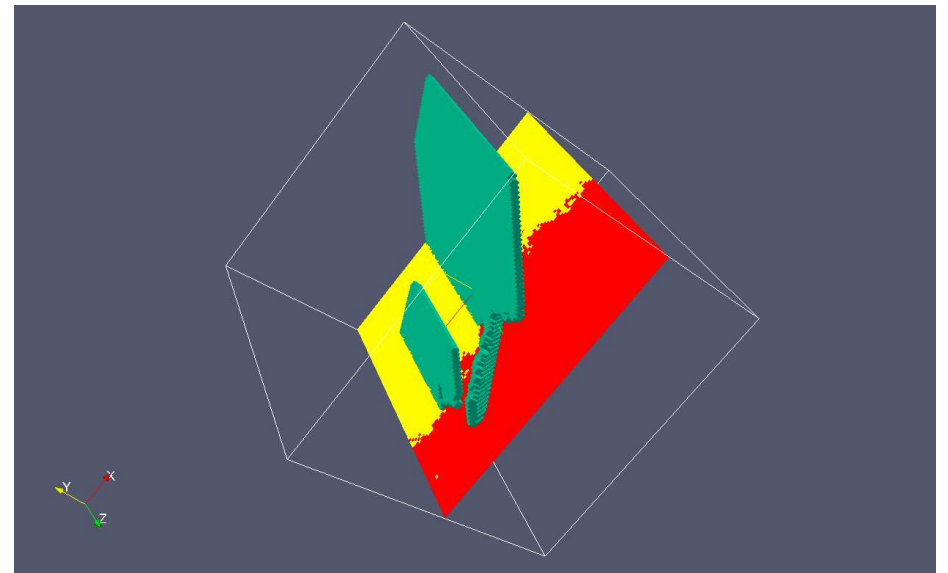
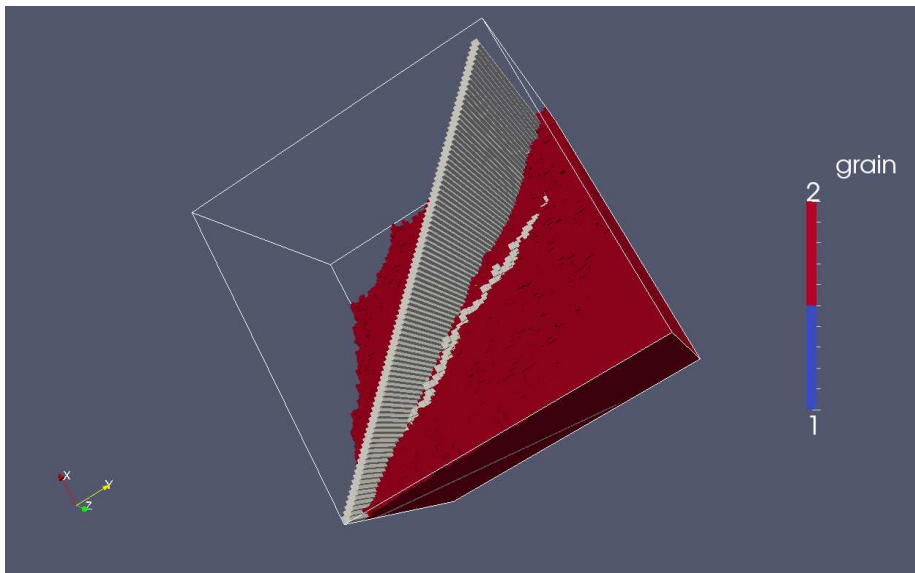
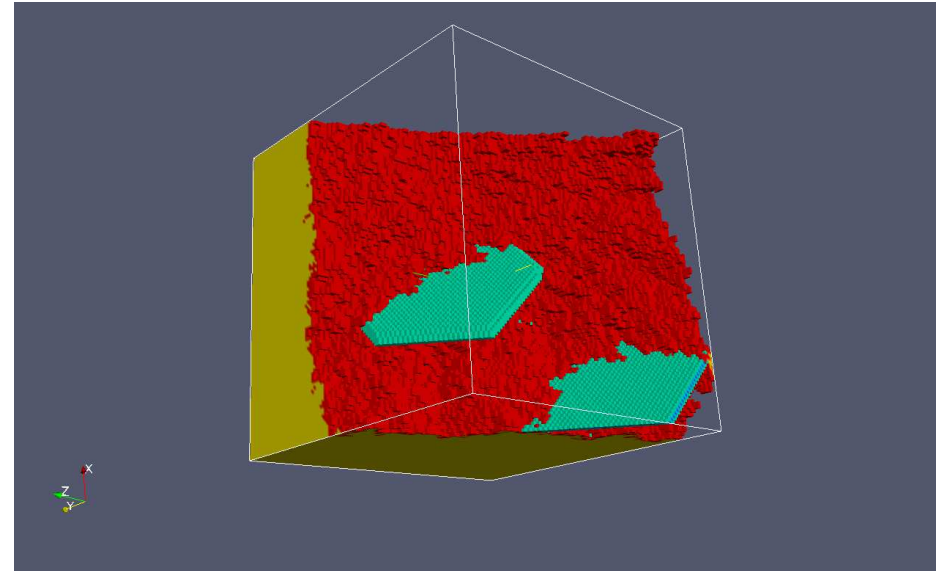
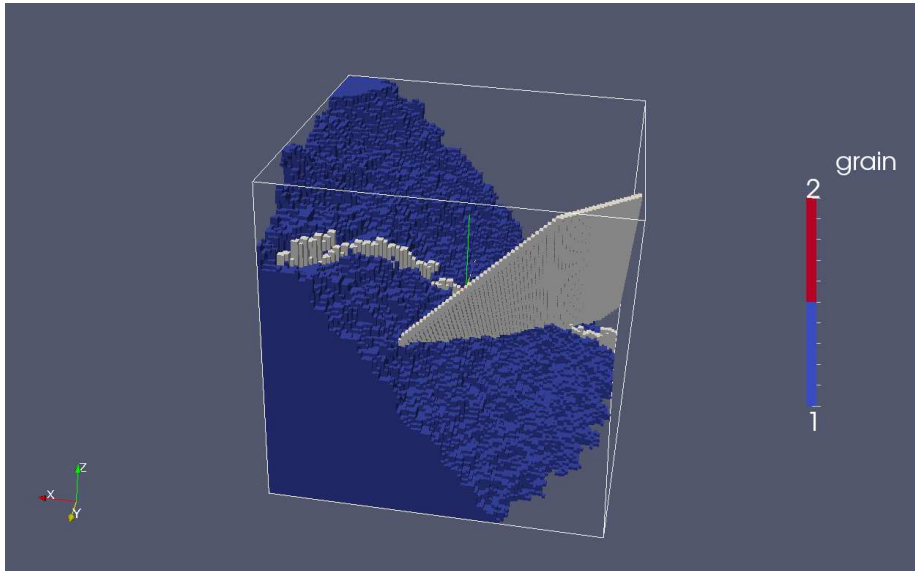
Grain boundaries



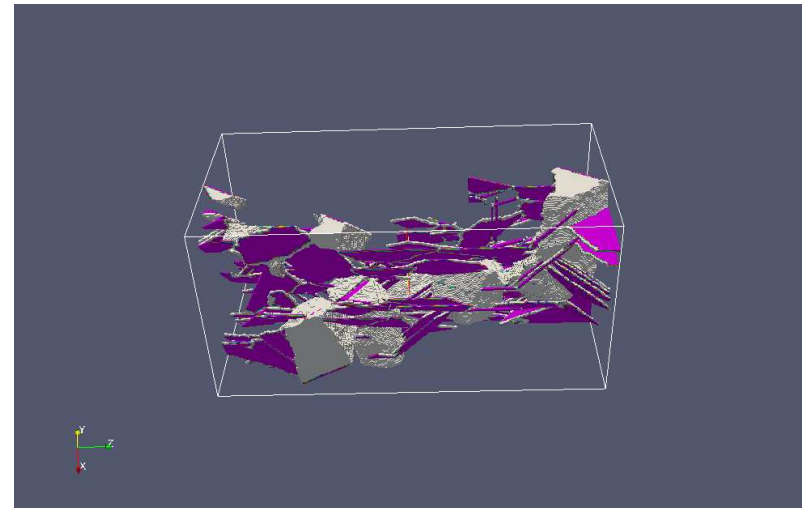
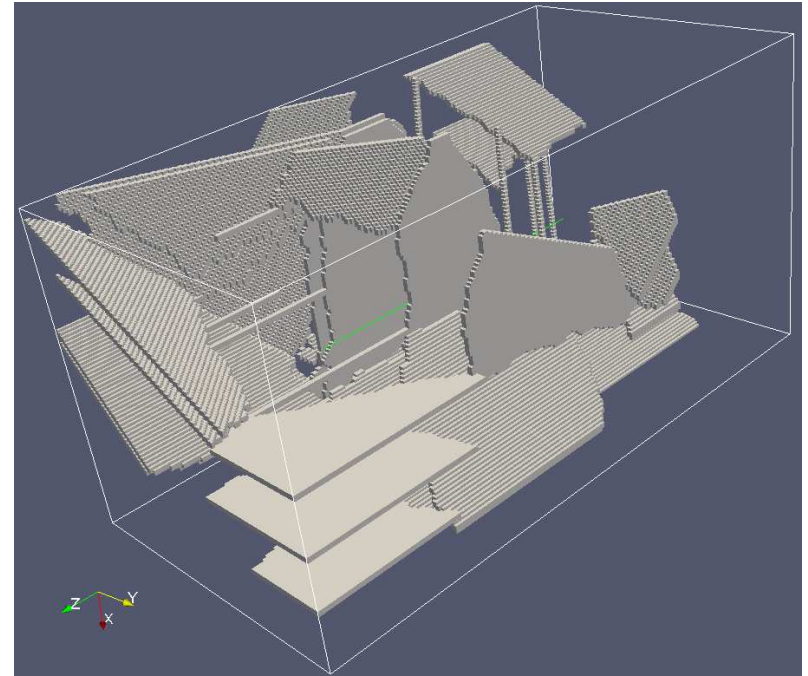
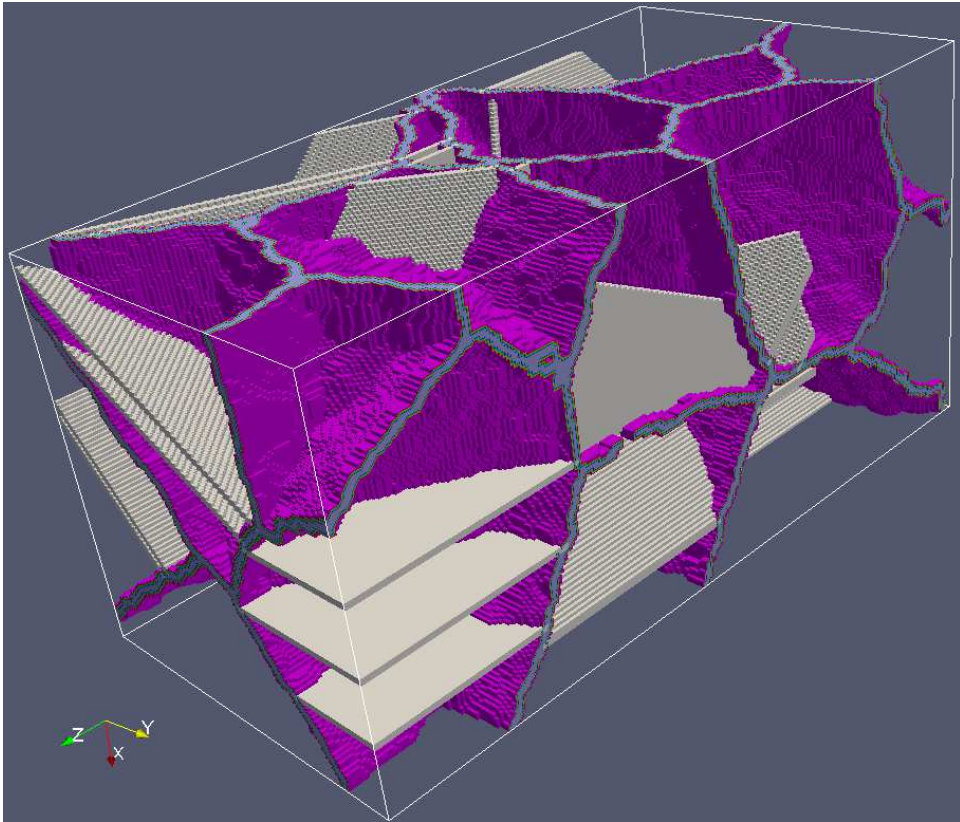
Grain boundaries



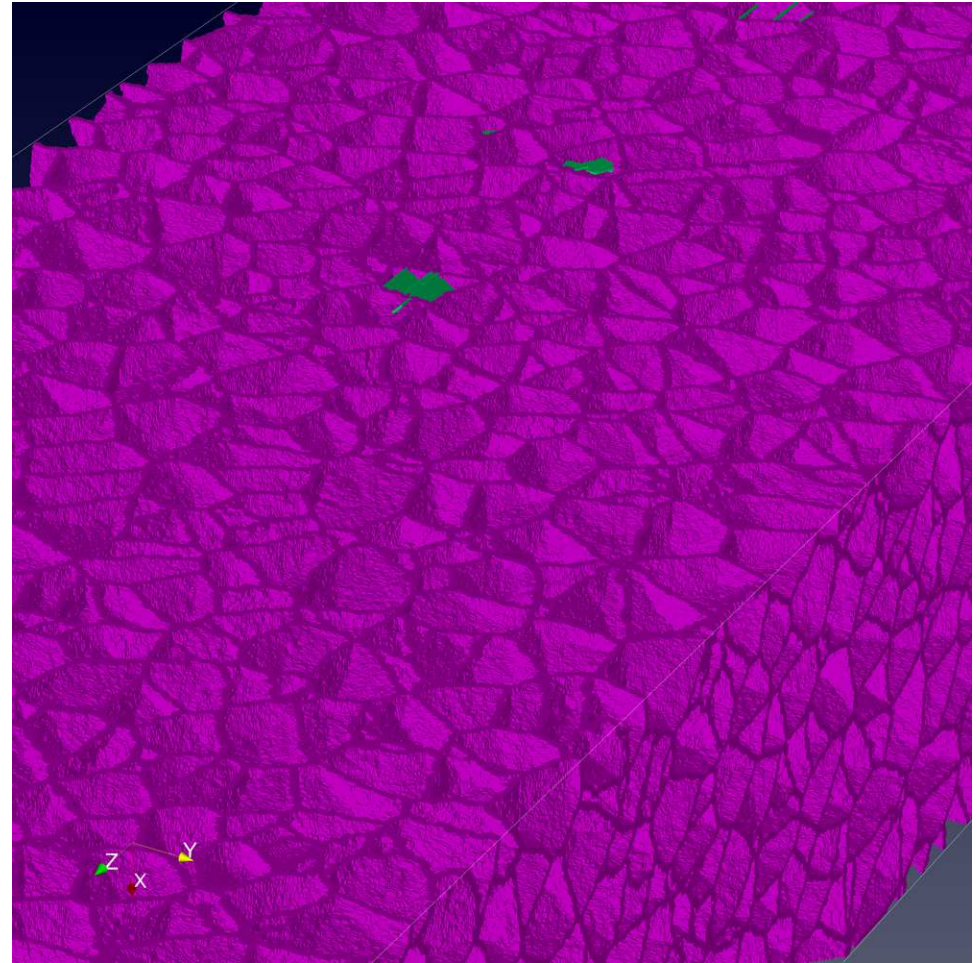
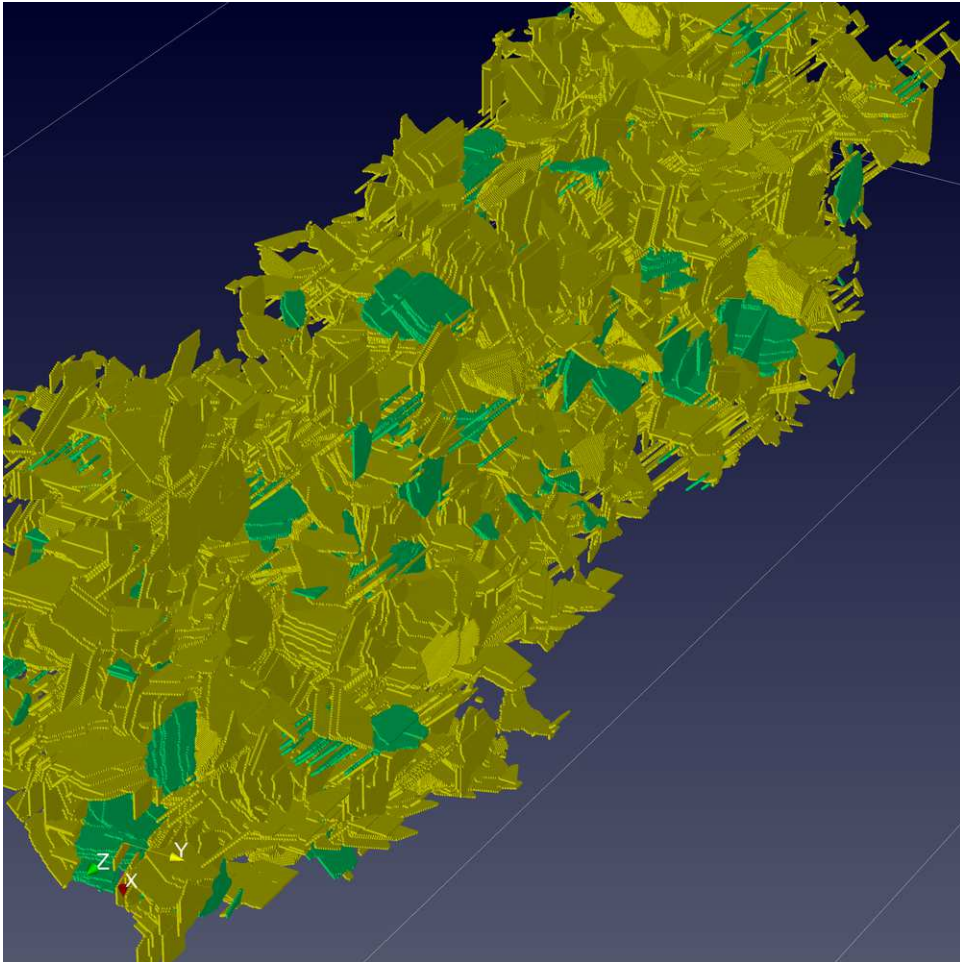
9. Cracks crossing GB



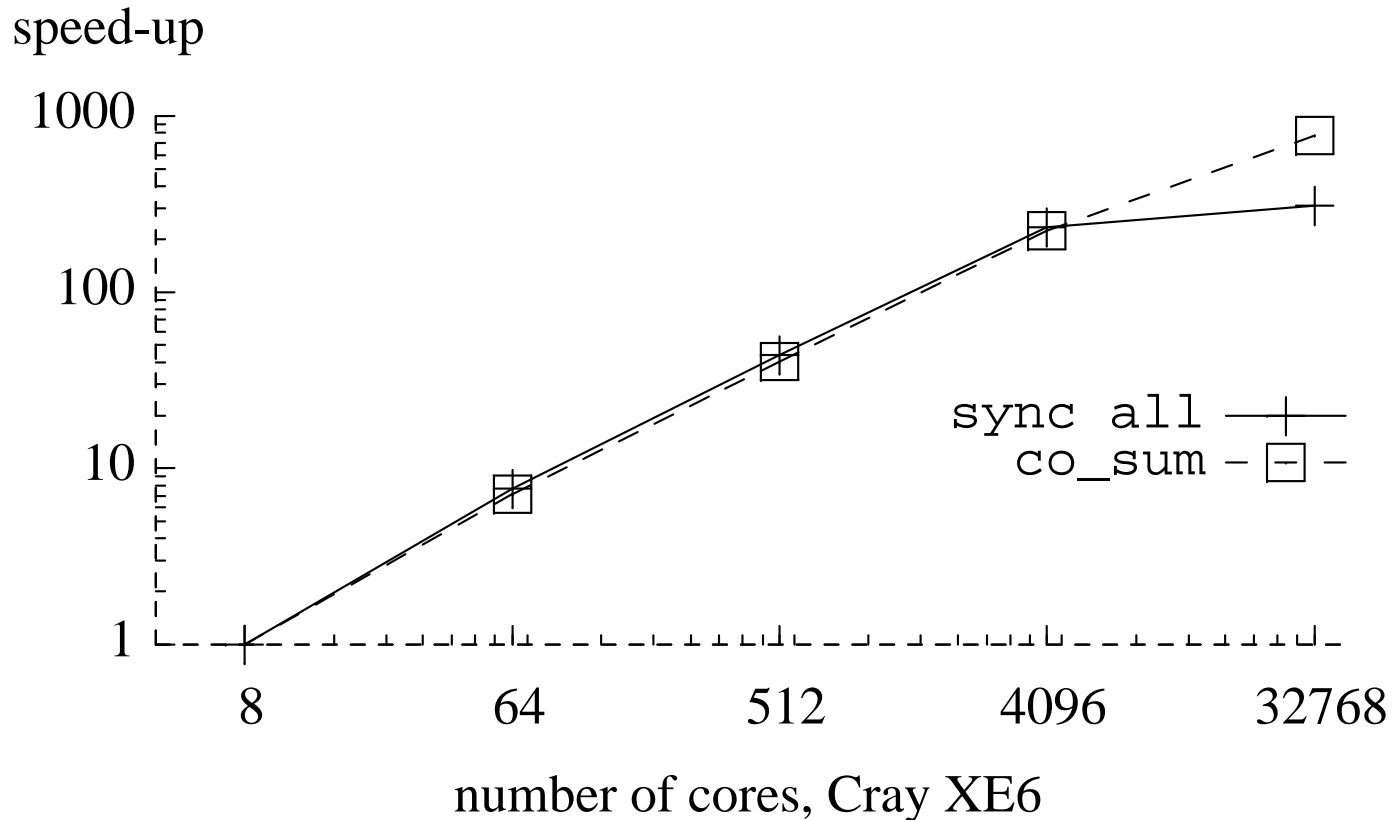
10. Microcracks joining into a macrocrack



Microcracks joining into a macrocrack, 10^9 cells



11. CA performance, Cray XE6, 10^9 cells¹⁶



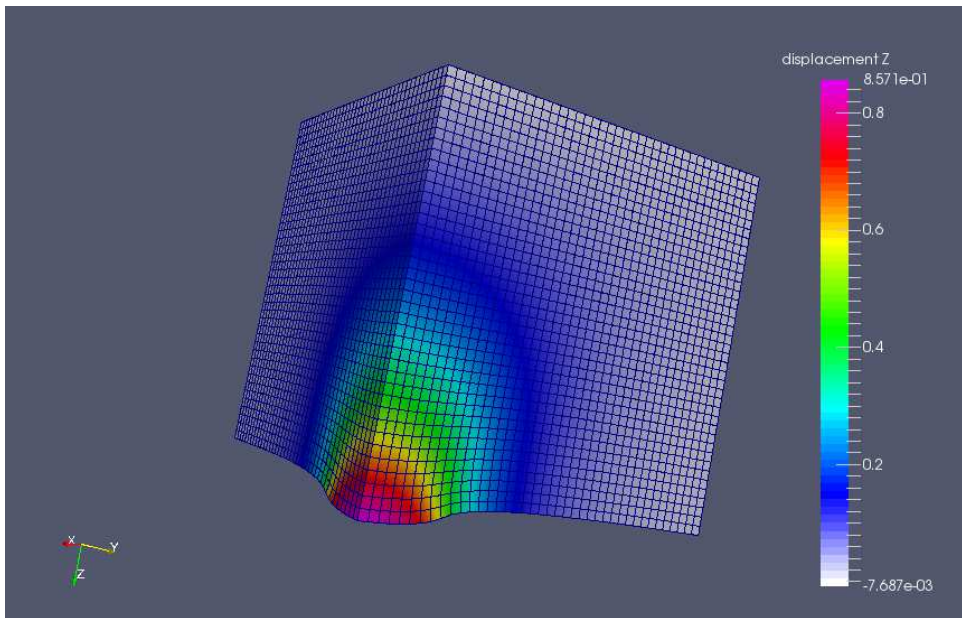
- Scaling due to identical calculations performed for all cells
- No asynchronous execution

12. CAFE sample results¹⁵

- 3D cube, quasi-static tension
- D , the CA damage variable per FE, $D = 1$ - no damage (intact), $D = 0$ - failed
- Update the Young's modulus:

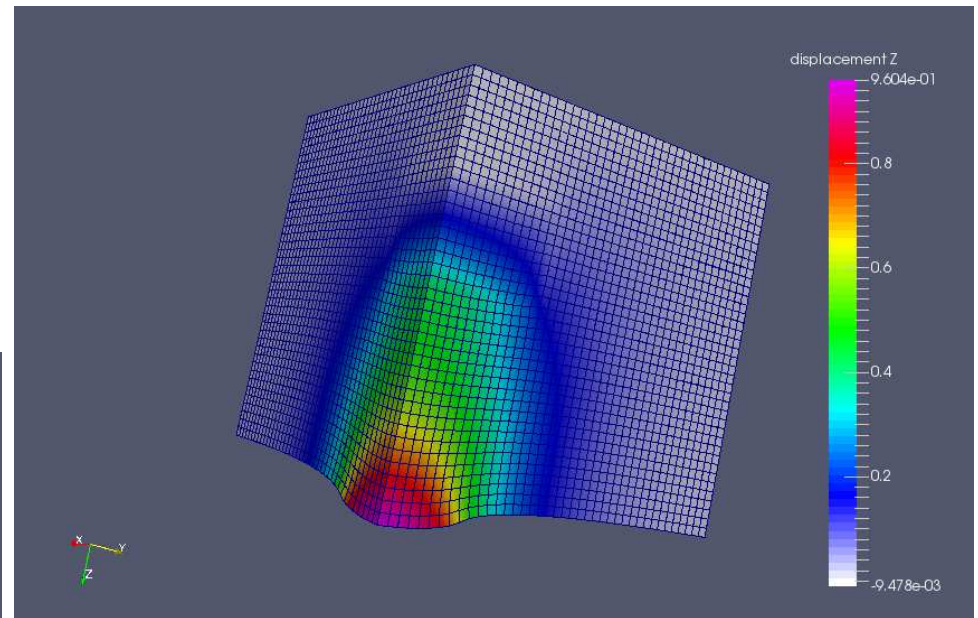
$$E = E_0 \times D$$

No cracking

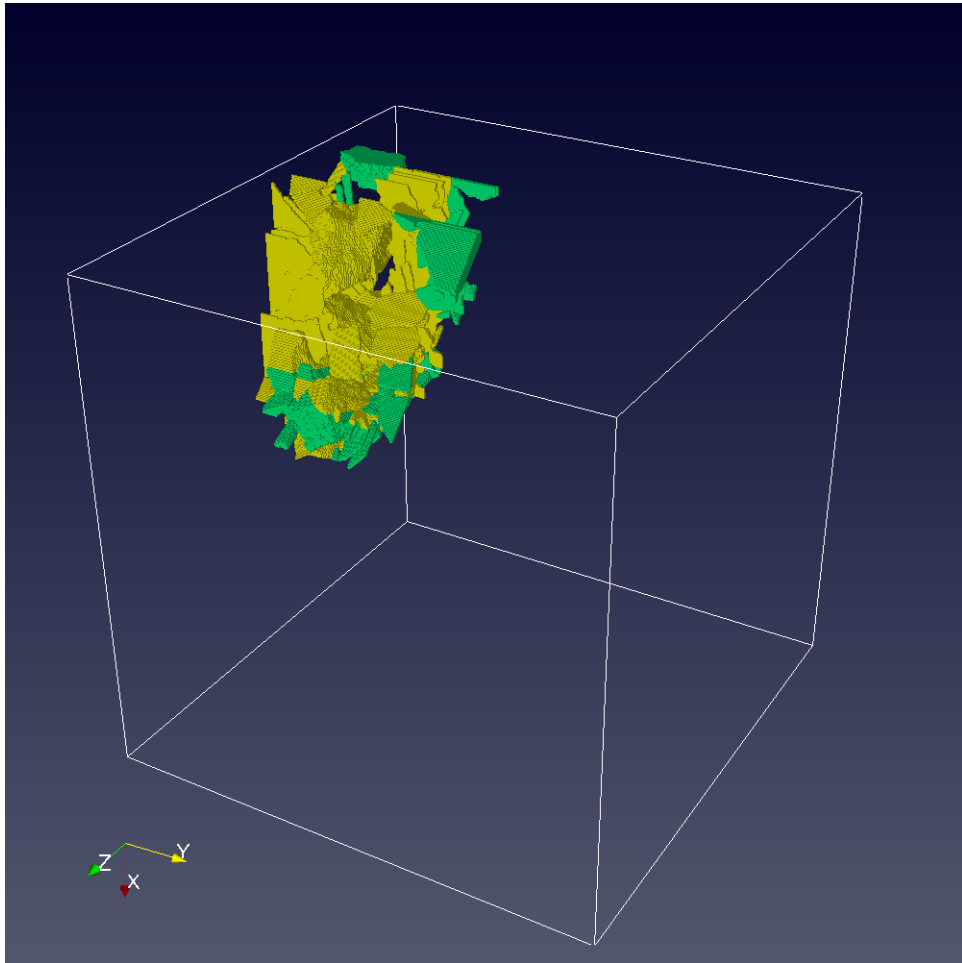


Cracked model

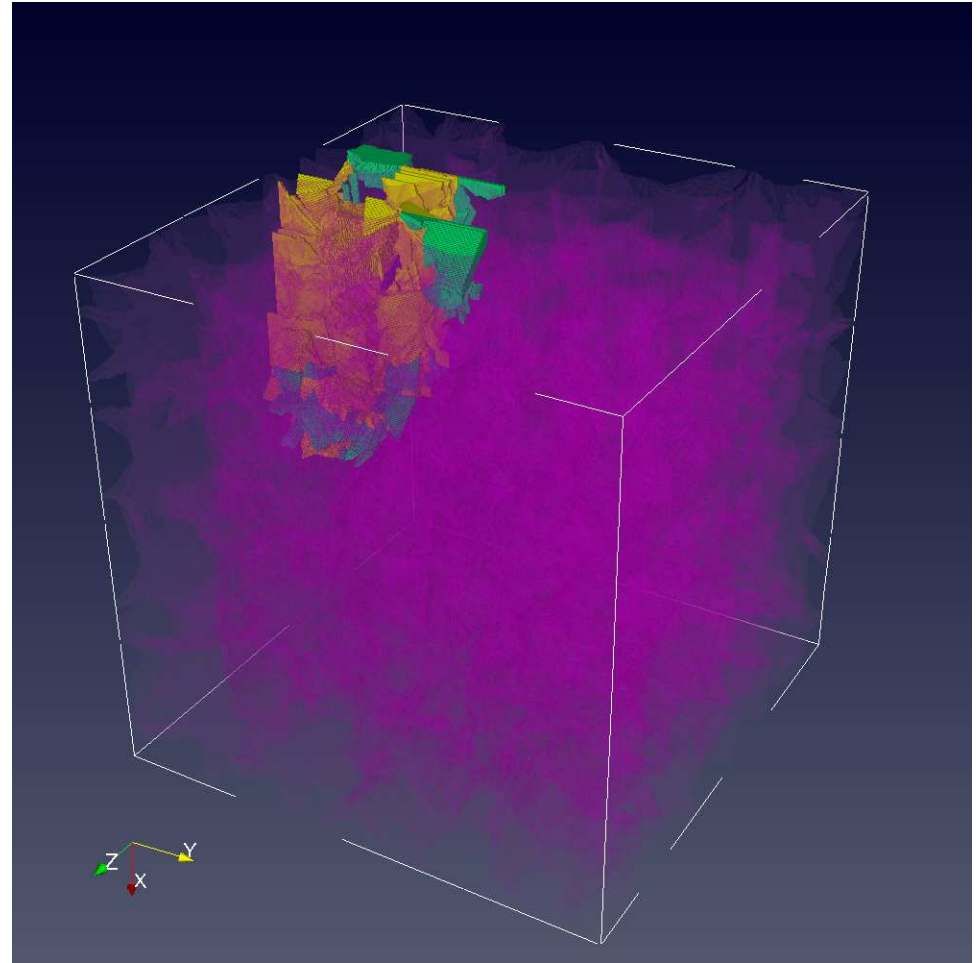
Note discontinuity on the blue band, corresponding to crack front crossing the boundary.



CAFE sample results



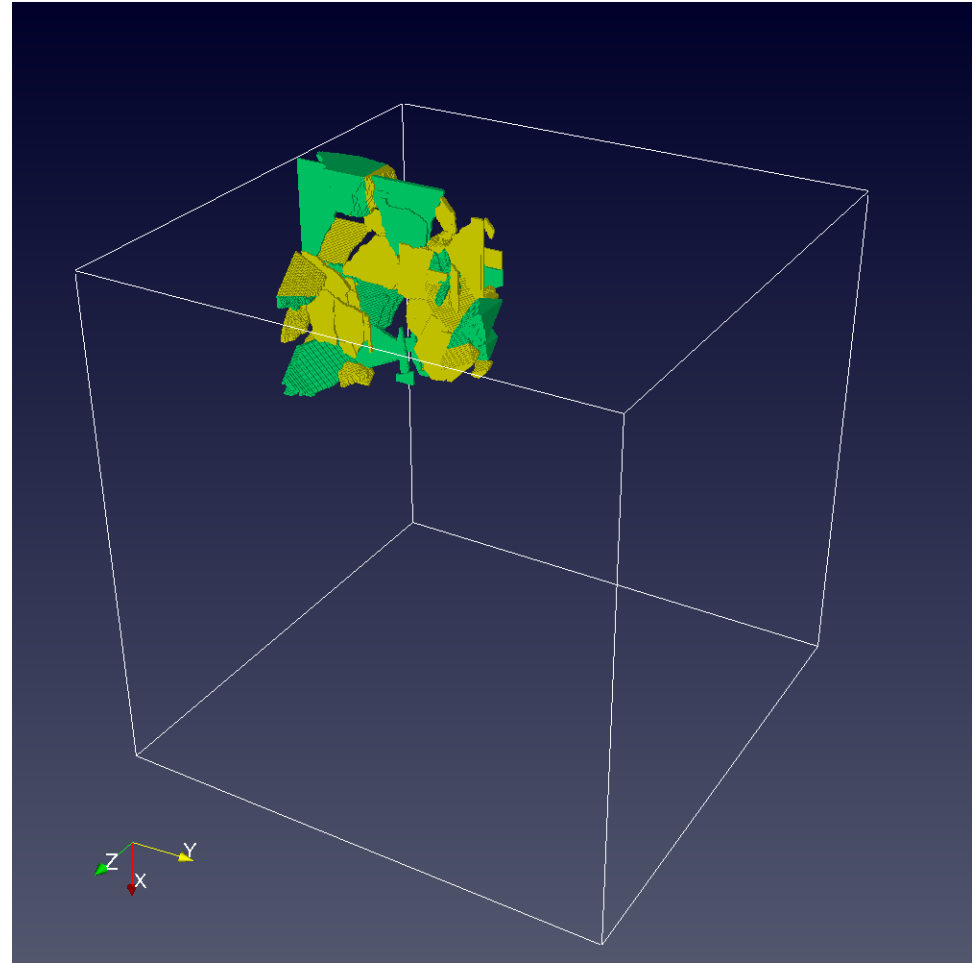
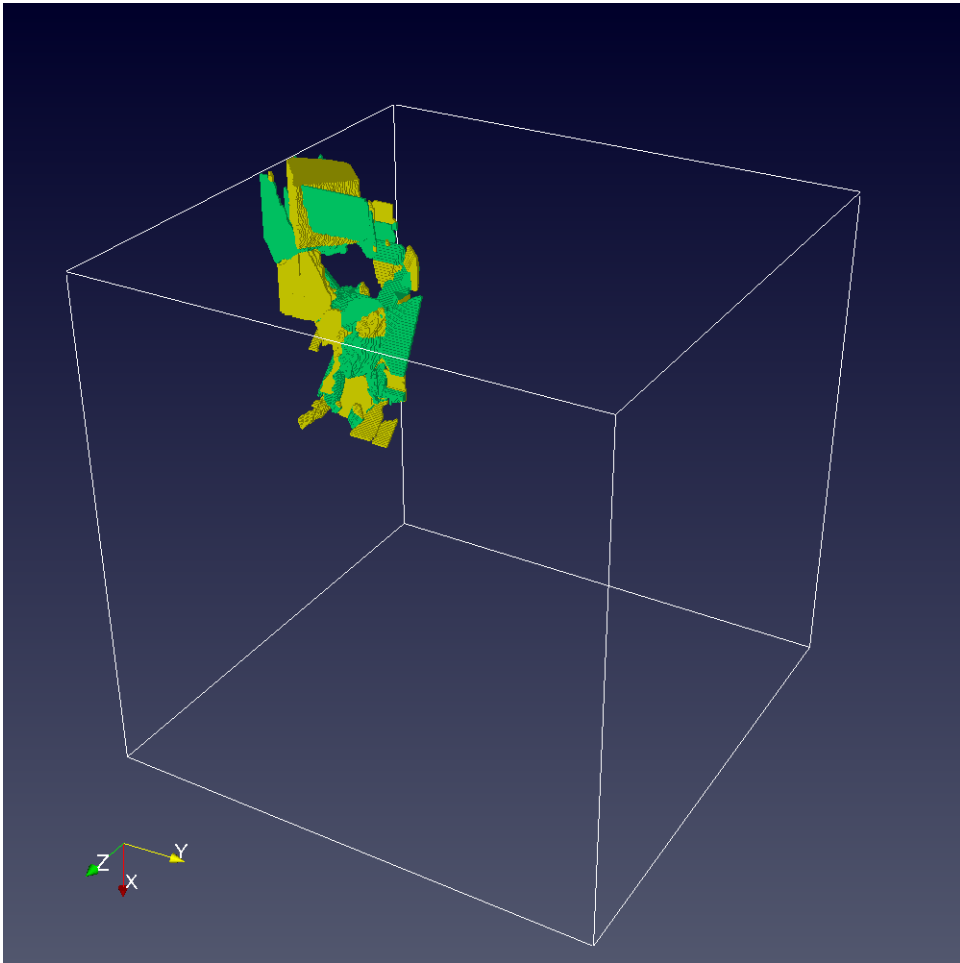
The macro-crack emerges as cleavage cracks in individual grains join up after crossing grain boundaries in poly-crystalline bcc iron. Green cracks - $\{110\}$ planes, yellow - $\{100\}$ planes.



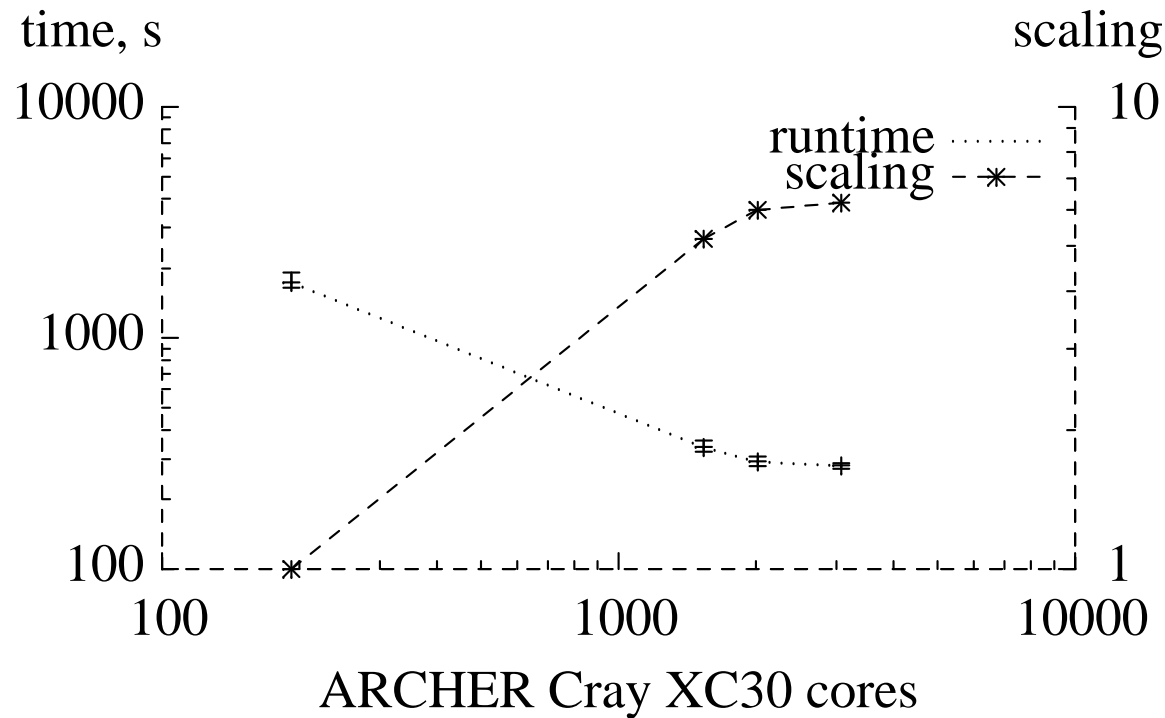
The process is driven by the FE stress fields on the macro-scale.

CAFE sample results, exploring uncertainty and scatter

Random samples of microstructure produce different crack paths.



13. ParaFEM/CGPACK CAFE scaling on ARCHER, Cray XC30



- 200 \rightarrow 1,500 cores = $\times 5$ scaling. Parallel efficiency of $> 60\%$.
- ParaFEM - MPI, CA - CGPACK - Fortran 2008 coarrays
- Hybrid MPI/coarray - novel, risky
- Cray and Intel now, GCC soon

14. Future: generic framework

We need:

- *Framework* for building multi-scale solid mechanics models
- *Flexible, expandable*- wide range of problems.
- *API* centred
- Opportunities for *code replacement* and *interoperability*.
- The framework must not be linked to any particular FE code or any particular microstructure model.
- *Concurrent* simulation at all scales, with a two way information exchange.¹⁸
- The framework must allow for implementing *homogenisation* and *localisation* (upscaling/downscaling) algorithms, e.g. using the representative volume of material (RVE)¹⁹ or nested homogenisation-localisation.²⁰
- Multi-scale models are large. *Petascale* now and *exascale* soon.
- The aim of the framework is to allow researchers to combine their micro- or mesa-scale models with a variety of continuum mechanics FE solvers.
- *Comparison* of different multi-scale models and of different modelling results will be more rigorous and fair.

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